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CHEMOGRAPHY CONCEPT IN CHEMICAL SPACE ANALYSIS

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Chemical space can be viewed as being analogous to the cosmological universe in its vastness, with chemical compounds populating space instead of stars. About 70 million compounds recorded in public databases represent still a very small portion of chemical universe estimated as ~ 10^{33} drug-like molecules [1] which could potentially be synthesized. *Chemography* is a relatively new field dealing with visualization of chemical data, representation of chemical space and navigation in this space. This may help chemist to choose compounds to be purchased or synthesized in order to enrich "in-house" databases, to select subsets for screening campaigns, and to predict chemical properties or biological activities of novel compounds. Chemography involves mapping of compounds into multi-dimensional space defined by molecular descriptors followed by the dimensionality reduction to 2 or 3 dimensions for visualization purposes.

This presentation focussess on the Generative Topographic Mapping (GTM) approach [2-5] which could efficiently be used to visualize different chemical spaces, to predict activity profiles, to conduct virtual screening and to compare large databases of chemical compounds.

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